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## A Workflow to Investigate Exposure and Pharmacokinetic Influences on High-Throughput in Vitro Chemical Screening Based on Adverse Outcome Pathways

Martin B. Phillips, Jeremy A. Leonard, Christopher M. Grulke, Daniel T. Chang, Stephen W. Edwards, Raina Brooks, Michael-Rock Goldsmith, Hisham El-Masri, and Yu-Mei Tan

Methods for ToxCast<sup>TM</sup> protocol

Chemical quality control

Chemical assays

References

**Table S1.** Structural similarities between "high priority" active chemicals and twenty-two remaining nearest neighbor inactive chemicals as determined through the presence or absence of structural Molecular Access System (MACCS) keys.